MANHaptic: A Haptic Adaptive Method for Precise Manipulation, Assembly and Navigation

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Many techniques may be applied to overcome the physical limitations induced by the small workspace of most haptic devices in a navigational context, such as the Bubble technique, or to manipulate virtual objects, such as clutching techniques. Several assembly tasks require high precision, and haptic-guide based approaches are often used in order to help the user to reach a precise and predefined assembly goal. However, there are a few haptic interaction techniques designed to facilitate micro-assembly tasks for which haptic guidance is unsuitable, such as protein docking. The objective is to find an optimal but precise 3D configuration by interactive exploration. In this paper, we propose an innovative technique to both overcome the physical limitations of the device and to reach the high accuracy required by micromanipulation tasks without a predefined goal. This approach is based on a non-isomorphic mapping around a neutral referential retrieved by an elastic haptic feedback, in addition to external haptic feedback. We present at the end of this paper an application and a preliminary ergonomic study of this approach in a molecular docking application framework.

Keywords: Virtual Reality; Haptic; Micro-Assembly.

I. Introduction

In Virtual Reality applications, haptic devices are used for manipulation and assembly tasks. Collision feedback rendered by 6 Degrees of Freedom (6DoF) haptic arms helps users to assemble 3D objects. Using haptic interaction for 3D object manipulation and assembly has a large range of applications in industry at different scales, from automotive to molecular design. However, all haptic devices have a limited workspace, a limited precision, and limited rotational movements. In order to overcome the limitations, a basic manipulation control is the clutching interaction technique, which is however time consuming and does not allow user to focus on his task. Several approaches use haptic device to control navigation during interaction [9], which uses the relative position of an object of interest, the position of the haptic device, and the user position, to compute a more suitable point of view for the user to interact with the object. Other solutions avoiding clutching/declutching, such as the Bubble technique [4], or the Haptic Hybrid Rotation method [5], propose to perceive (via haptic and visual rendering) the hardware limitations of the haptic device, and provide a rate control used for manipulation, based on an isomorphic mapping when the device is far from its workspace boundaries, and on a non-isomorphic mapping near the boundaries [10][8], On the contrary to these methods based on the haptic workspace boundaries, the MAN- Haptic approach is based on a *neutral referential*, as in [7], [3] or [6]. Our approach allows combining 6DoF elastic force feedback to retrieve this neutral referential and external feedback such as collisions, and uses a non-isomorphic rate control based on this neutral referential for manipulation. In this paper, we describe this innovative approach especially designed for micromanipulation features needed in haptic molecular docking applications. Then we present a preliminary ergonomic studies performed in order to validate this interaction method, before a discussion and a conclusion about this work.

II. MANHAPTIC TECHNIQUE

A. Concept

Our solution is an implementation of a rate control technique with a 6DoF feedback device, based on a neutral referential is defined according to the convenience of the user, with provides also feed-back force and torque bringing the device back to this referential. The interpolation of movement is obtained by a downscale factor for translation and by a quaternion interpolation for rotation. The level of interpolation varies according to the distance of the two objects to be assembled. We also focus on maintaining the coherence with the collision forces generated by the interaction of the object with the rest of the scene.

B. Retrieving an Haptic Neutral Referential Using Elas- tic Force Feedback

Rate control systems imply the existence of a fixed neutral position/orientation on the device where a null rate is applied. Retrieving this position must be easy and convenient for the user. Elastic devices are generally more suitable for rate control paradigms because they automatically retrieve the original position [12]. Here, we will use the force feedback to simulate the elastic forces needed to return to a given position/orientation. First, we define a neutral referential with an origin corresponding to the most convenient position/orientation for the user holding the device. This is inspired from a 6DoF control mode proposed to navigate in a virtual world [3]. The referential is determined by software calibration. For each movement, we calculate a feedback force and torque to bring the user back to this neutral orientation/position (see Figure 1.). In order to compensate the inherent imprecisions of the device, we define a "dead zone" near the neutral referential, in which no movement occurs. The device is then physically restrained inside a comfortable workspace, while the virtual objects have an infinite motion space.

$!S = !p \ ! \ i$ (1)
$qs = qd \ ! \ qo$ (2)
$qa = slerp(q0, qs, t)$ (3)

C. Interpolation

Concerning translational motion, the interpolation is done by rescaling the distance position vector device from the origin of the neutral referential. In the following equation, $!S$ is the interpolated translation, $!p$ the current device's vector position and i the scaling factor. Concerning rotation, at any time of the manipulation, the rotational motion of the device controls the angular velocity of the object. The orientations of the device qd and the object qo are represented by quaternions. The rotational motion *qs* of the object is then given by the multiplication of the two quaternions (see Figure 1.). The SLERP interpolation [11] is traditionally used to calculate intermediate frames between two quaternions (start and end orientations) in order to produce smooth animations. Here, we use the SLERP interpolation to calculate a range of quaternion orientations, between the current object's orientation and the one it would adopt after the motion. Then, an orientation at the time t can be picked according to the desired level of attenuation. In the following equation, qs is the quaternion representing the rotational motion applied to the object without interpolation, qd is the quaternion of the device and qo the quaternion of the object. qa is the softened speed using the *SLERP* function applied between qo and qs at the time *t* of the interpolation. Here, t and i are functions of the distance between the manipulated object and the area of assembly. The attenuation increases when this distance decreases.

D. Scene and Rate Control Feedback Coherence

The interaction between the bound object and the rest of the scene produces collision forces. These forces are not directly applied to the object in the scene, but are rendered by a haptic force-feedback summed with the elastic feedback used to retrieve the neutral referential. The feedback loop (see Figure 2.4) ensures the coherence of these force. When the user moves the object into another one, the associated feedback

force and torque oblige the user to trans- late/rotate to a position/orientation in which there is no more collision. Meanwhile, the rotational feedback torque is acting and obliges the user to bring the device back in the deadzone, which stops the object's rotation when no collision occurs anymore.

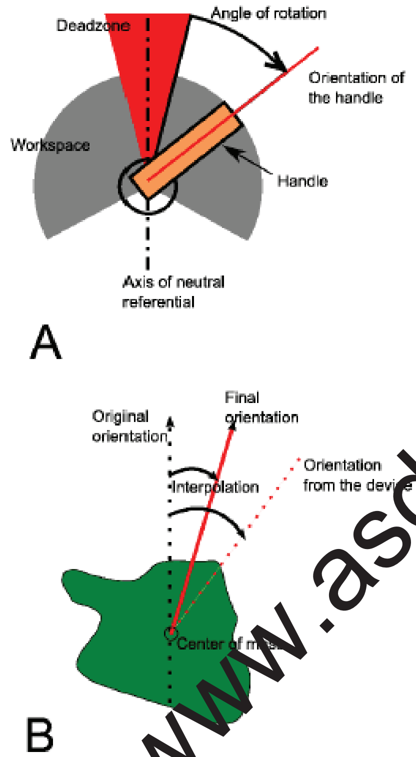

Figure 1. Results of a device rotation.

A, the device is rotated from the axis of the neutral referential to the orientation r, taking into account the dead zone. The retrieval torque R is thus equal to –r. B, the motion of the device is mapped on the object, qo representing the neutral referential. The final orientation qa is obtained by applying the SLERP interpolation.

III. Application: Molecular Docking

The motivation for this new technique has come from the need to manipulate proteins in a docking application using a 6DoF device.

A. Overview of the application

Protein docking aims at assembling two molecules according to a lock and key principle. It is a computational method designed to predict the position and orientation of a protein ligand (key) when bound to a protein receptor (lock), taking into account physical and chemical properties. This approach is intensively used in biological and pharmaceutical research. Data resulting from an automated protein docking procedure allows numerical analysis and graphical simulation of protein movements. However, such an approach is computationally expensive and can produce irrelevant predictions. The purpose of the VR molecular docking application is to propose interactive simulations in which the researcher can virtually explore the proteins. Drawing benefit from the user's experience, subsequent computational docking methods can be focused on interesting cases. Virtual molecular docking is similar to virtual assembly tasks, but with sometimes very complex surfaces. One of the challenges lies in the protein manipulation

paradigm. We developed the new MANhaptic method to provide a fine control of the protein with a 6DoF force-feedback device. While the application provides precise physical and chemical information during the manipulation, this paper focuses only on the collision model that renders an overall force summed with the elastic feedback used to retrieve the neutral referential.

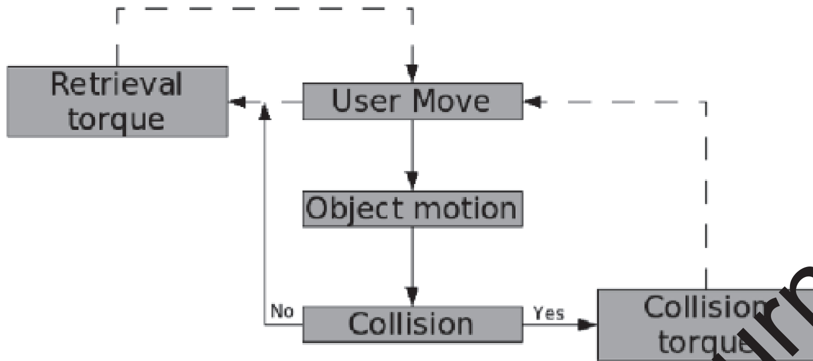

Figure 2. Feedback loop. The dashed lines represent force- feedback.

IV. Evaluation

In this paper, the evaluation focuses on rotational movements. The paradigm could be applied to translation, but we had no need to do so because the scale of the virtual scene was easily adjusted to the device workspace and the size of the objects does not require big translational moves, assuming they are placed near each other at the beginning. The MAN haptic technique for rotations paradigm was evaluated during an interactive molecular docking experiment. In each trial we asked the participants to reproduce a given assembly of two molecules as accurately as possible. To analyze this experiment, we recorded the performance of the participants by recording completion time and accuracy of the assembly compared with the solution. At the end, we collected data about subjective criteria.

A. Participants

Ten participants took part in this preliminary experiment. They were aged from 22 to 40 years. All of them were right handed and they did not have any knowledge in molecular modeling or docking. The experiment comprised two sessions: one for the clutching technique, one for the MANhaptic technique. One half of the participants started with clutching first, and the other half with the MANhaptic technique first. The second session took place a few days after the first one, in order to minimize learning effects.

B. Experimental Apparatus

The experiment was leaded on a 6DoF (input and output) haptic device. The simulation and visualisation framework was based on a homemade interactive protein docking application. The contacts were rendered as described in section 4.2 and coupled with our MANHaptic technique. Four trials presented a scene showing two independent 3D objects in the middle of the screen and the assembly solution in the upper right corner. The device was directly bound to one of the objects. Each trial corresponds to one type of assembly: a cone in a hole, a thin object filling a slot, two matching surfaces and a real molecule docking case (respectively A, B, C and D in Figure 3.). The first three were geometrical 3D assemblies. They were built by placing points in space coordinates. These points are considered as atoms by our application, which is able to treat them as molecules. The last trial consists in reproducing the assembly of a real protein complex, namely 1CTA referenced in the *Protein Data Bank* (PDB).

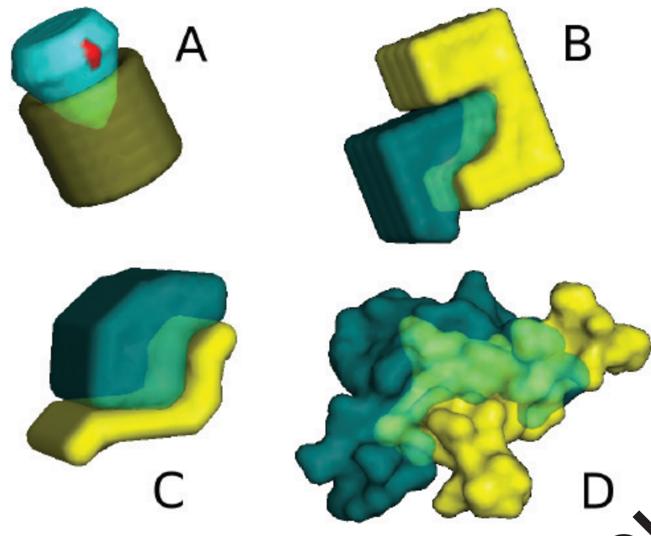

Figure 3. From simple assembly to complex protein assemby

C. Compared Techniques

We compared our rotational technique with the classical clutching approach. For translation, we chose to use position control with no scaling factors in both cases. To do so, we matched the virtual space and the physical workspace of the haptic device.

1) Clutching

When the user is physically stopped in his movement, by reaching either a boundary of the device or an uncomfortable wrist position, he can press the clutching button to find a better position without moving the virtual object. When releasing, the object is re-attached with the same position and orientation. The motion of the object is position controlled.

2) Rate Control based on neutral referential

We implemented the rate control as described in section 3 of this paper. The neutral referential was defined at the beginning of the trial. We let each participant choose the most comfortable position and calibrated it in the program. The dead zone was a set of cones around each axis with an 8.5 Ångström radius. This measure was empirically established to compensate the imprecision of the device.

3) Procedure

The participant stands in front of the screen and slightly on the left of the device (on the right in the case of a lefthanded individual). Once the user is comfortably positioned, we calibrate the neutral referential. The experiment begins with a training phase during which we provide instructions about the experiment and how to operate the device. The scene is composed of two objects. The participant manipulates the blue one called the ligand. The yellow one (the receptor) is fixed in space. At any moment the subject can press a button on the device to enter in a view mode. Then both objects can be rotated around the center of mass of the receptor, keeping the same relative distance and orientation for both objects. Pressing the button again, switches back to the control mode keeping the new view. There is no time limit to become familiar with the device, the objects and how they interact. Then follow four trials in which the goal is to assemble two molecules as in a solution presented in the upper right corner of the scene. The receptor in the solution has always the same orientation as the one in the scene. The participant clearly sees how the ligand must be docked whatever the angle of view chosen in view mode.

4) Data

For each trial we recorded the completion time and the accuracy of the assembly in comparison with the solution. The measure of the completion time, in seconds, starts when the participant grasps the device's handle. It ends when he presses the validation but- ton. Concerning the accuracy of the assembly, when the subject validates, his assembly is aligned with the solution by overlaying the manipulated receptor onto the one in the solution. Then, the program computes the Root Mean Square Deviation (RMSD) between the respective atoms of the two ligands. This is the sum of the distances of each pair of atoms divided by the number of pairs. A perfect match is indicated by a score of 0, meaning no deviation occurs. In addition to these measures, each participant took the Mental Rotation Test [1] and, at the end of the experiment, he/she was asked for a subjective global appreciation about the technique. After the second session, the participants were asked to rank each technique from 1 to 5, 5 being the top mark.

5) Results

Four classes of participants were defined according to their results on the MRT. The first class were subjects who scored from 0 to 5 (10%), the second from 6 to 10 (30%), the third from 11 to 15 (40%) and the fourth from 16 to 20 (20%). Those in class four are supposed to obtain the best performance. We computed Kendall correlation coefficients on the completion time (z=1.14, n.s.) and accuracy (z=0.83, n.s.), which show no correlation between these variables and the MRT results. Then performances of participants were analyzed through a Multivariate Analysis of Variance (MANOVA) on completion time and accuracy of the assembly. The manipulation technique was the distinctive factor between subjects. The results for completion time and accuracy (see Table *1*) seems to indicate that there is no significant effect according to the technique used. This is confirmed by the Wilks test. Moreover, ANOVA were performed on the subjective appreciation of participants about the different techniques (see Table *1*). The mean rank of the MANhaptic technique is slightly better than the one of clutching. The statistical test shows no significance.

	Clutching	MANhaptic	
Completion time (s)	*m = [illegible]98.8* *sd = 152.8*	*m = 225.9* *sd = 199.8*	Wilks test *Lambda = 0.993* *F = 0.113* *n.s.*
Accuracy (RMSD in Å)	*m = 0.685* *sd = 0.454*	*m = 0.731* *sd = 0.531*	
Subjective ranking	*m = 3.0* *sd = 0.82*	*m = 3.6* *sd = 0.96*	ANOVA test *F = 2.25* *p = 0.151* *n.s.*

Table 1. Results of the assembly tasks in terms of completion time, accuracy and subjective ranking.

D. Discussion

This evaluation shows that our *MANhaptic* approach does not decrease the performance of the manipulation compared with the classical clutching technique. Indeed, no significant effects on the completion time were observed. However we have to highlight the fact in our paradigm, that rotational decrease with the distance of the two objects that makes difficult to compare performance in term of completion time.

Accuracy showed comparable performance too. Concerning the subjective appreciation, in spite of a slightly better ranking of the MANhaptic technique, a statistical test does not rate the difference as significant. Nevertheless, in general remarks user feeling according to the docking task were in favor of our technique. Participants found the MANhaptic technique less disturbing than clutching, appreciating the fact that there is no button to press to manipulate the object. Furthermore, their arm was never in an uncomfortable posture. They furthermore liked the adaptive interpolation. The slowness of the interaction when the two

objects are very close was judged pertinent in order to accurately assemble the objects. Another interesting observation is that the most negative comments were not about the manipulation technique itself, but about difficulties about the 3D visual perception of the complex protein surfaces (see figure 3 D).

This paper describes a non-isomorphic mapping approach, using quaternion representation and SLERP function, to address the issue of micromanipulation with a haptic 6DoF device. The variations in position and orientation of the device, with respect to a neutral referential chosen by the user, are used to compute the rotational and translational interpolation. In addition, an elastic haptic feedback is provided to help the user recover the neutral referential. Such an approach allows continuous rendering of external feedback computed from the collision between the atoms of the two molecules to assemble in our case. Finally, we presented the results of an ergonomic study that was carried out on our approach in the framework of a molecular docking application. According to the results of the ergonomic study, our technique provides at least the same precision (RMSD) and performance (task time) than direct manipulation with clutching/declutching and successfully overcomes the physical limitations of the device. Moreover subjective results show that users feel more comfortable with our method, which avoids the clutching mechanism. We suspect that these results come from the fact that the user is more focused on the assembly task, instead of spending time in clutching/declutching. Further evaluation must be lead in this way. Our approach could thus be an alternative to classical ones and provide at least the same efficiency. We are working on improving the precision of our approach by dynamically tuning the scaling factor used to control rotational and translational velocity. This could be done using the minimal distance between the two objects during the assembly. In further works, we will also provide an evaluation on applying this paradigm for navigation. We will especially evaluate whether our approach, providing haptic rotational and translational feedback to retrieve the neutral referential, could be more efficient than other tracking-based navigation techniques using a neutral referential as in [3], [6] or [7]. Finally, we highlight the fact that our approach addresses most problems of the physical limitations of haptic devices (workspace size, precision, mechanical constraints), avoids the use of a clutching/declutching mechanism, is well-adapted to both manipulation and navigation, could be applied on other 6DoF devices, and does not require complementary visual feedback.

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